Decision Trees

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The need for interpretability

How to maintain trust in AI

Beyond developing initial trust, however, creators of AI also must work to maintain that trust. Siau and Wang suggest seven ways of "developing continuous trust" beyond the initial phases of product development:

- Usability and reliability. AI "should be designed to operate easily and intuitively," Siau and Wang write. "There should be no unexpected downtime or crashes."
- Collaboration and communication. AI developers want to create systems that perform autonomously, without human involvement. Developers must focus on creating AI applications that smoothly and easily collaborate and communicate with humans.
- Sociability and bonding. Building social activities into AI applications is one way to strengthen trust. A robotic dog that can recognize its owner and show affection is one example, Siau and Wang write.
- Security and privacy protection. AI applications rely on large data sets, so ensuring privacy and security will be crucial to establishing trust in the applications.
- Interpretability. Just as transparency is instrumental in building initial trust, interpretability – or the ability for a machine to explain its conclusions or actions – will help sustain trust.

Training Data

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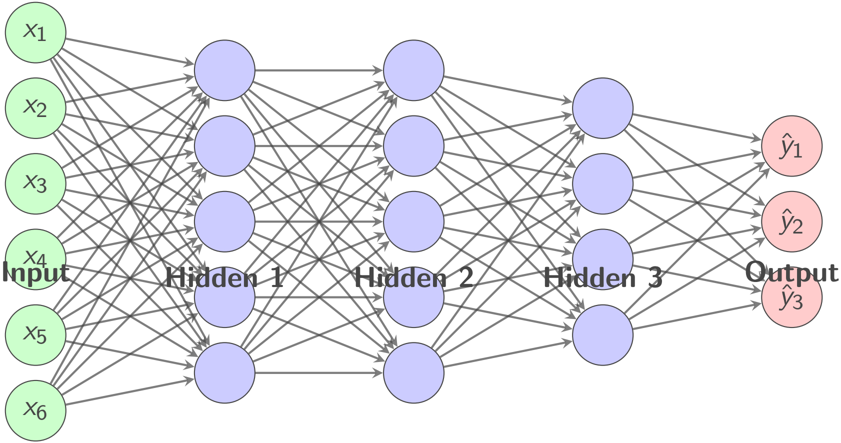
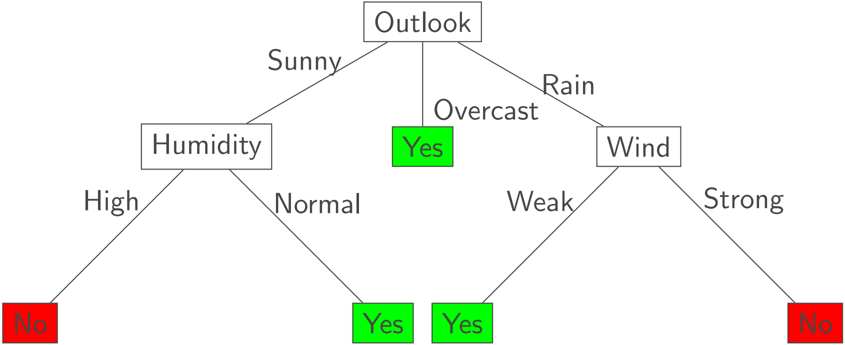
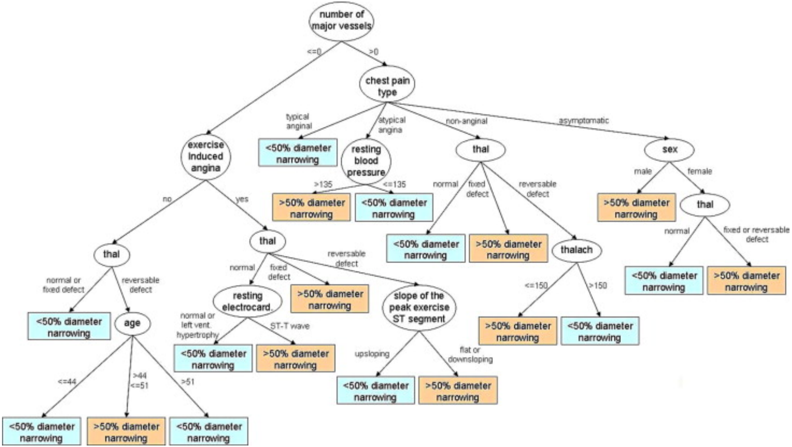
Learning a Complicated Neural Network



Learnt Decision Tree

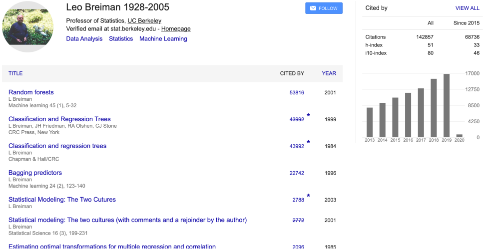


Medical Diagnosis using Decision Trees



Source: Improving medical decision trees by combining relevant health-care criteria

Leo Breiman (1928-2005)


Leo Breiman 1928-2005

FOLLOW

Professor of Statistics, UC Berkeley
Verified email at stat.berkeley.edu - Homepage
Data Analysis Statistics Machine Learning

TITLE	CITED BY	YEAR
Random forests L Breiman Machine learning 45 (1), 5-32	53816	2001
Classification and Regression Trees L Breiman, JH Friedman, RA Olshen, CJ Stone CRC Press, New York	~~43992~~ *	1999
Classification and regression trees L Breiman Chapman & Hall/CRC	43992 *	1984
Bagging predictors L Breiman Machine learning 24 (2), 123-140	22742	1996
Statistical Modeling: The Two Cutures L Breiman	2788 *	2003
Statistical modeling: The two cultures (with comments and a rejoinder by the author) L Breiman Statistical Science 16 (3), 199-231	~~2772~~	2001
Estimating optimal transformations for multiple regression and correlation	2096	1985

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Leo Breiman: Revolutionary Contributions to ML

Key Points

Major Algorithmic Breakthroughs:

- **CART (1984)**: Classification and Regression Trees

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- **Two Cultures (2001)**: Data modeling vs. algorithmic modeling

Computational Complexity Classes: A Quick Primer

Definition: Key Complexity Classes

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  - Example: Optimization versions of NP-Complete problems

Finding the Optimal Decision Tree

Volume 5, number 1 INFORMATION PROCESSING LETTERS May 1976

CONSTRUCTING OPTIMAL BINARY DECISION TREES IS NP-COMPLETE*

Laurent HYAFIL
IRIA – Laboria, 78150 Rocquencourt, France

and

Ronald L. RIVEST
Dept. of Electrical Engineering and Computer Science, M.I.T., Cambridge, Massachusetts 02139, USA

Received 7 November 1975, revised version received 26 January 1976

Binary decision trees, computational complexity, NP-complete

The Problem: Given training data, find the decision tree with highest accuracy

Optimal Decision Trees are NP-Complete

Important: Computational Complexity

Finding optimal decision tree is NP-Complete

- **Verification**: Given a tree, check its accuracy quickly ✓

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Example: What This Means

- No efficient algorithm exists (unless P = NP)
- Must use heuristics like greedy algorithms
- ID3, C4.5, CART use greedy approaches
- Good solutions, but no optimality guarantee

Greedy Algorithm

Core idea: At each level, choose an attribute that gives **biggest estimated** performance gain!

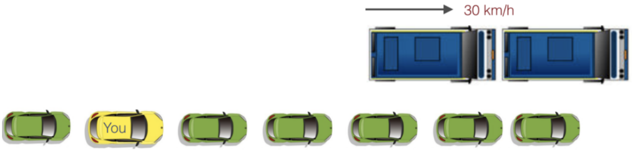

Image source: analyticsvidhya

Greedy $\neq$ Optimal

Towards biggest estimated performance gain

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- Need some statistical measure of "disagreement"

Claude Shannon (1948): The Birth of Information Theory

Definition: The Big Idea

Information is inversely related to probability. **Rare events are more informative!**

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Shannon's insight: The amount of information in an event should be inversely proportional to its probability.

Measuring Surprise: Step by Step

Shannon's Information Formula:

$$I(x) = -\log_2 p(x)$$

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Why base 2? So information is measured in **bits**.

Calculating Surprise: Detailed Examples

Example 1: Summer weather in Phoenix

- Sunny day: $p = 0.9$

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- Sunny day: $p = 0.9$
- Information: $I = -\log_2(0.9) = -(-0.152) = 0.152$ bits
- **Low surprise** - we expect sunny weather

Example 2: Snow in Phoenix in July

- Probability: $p = 0.0001$ (extremely rare!)
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Notice: Rare events carry $\sim 90\times$ more information!

From Single Events to Distributions

Question: What if we have multiple possible outcomes?

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Problem: Each day gives different amounts of information!

- If it's rainy: $I = -\log_2(0.5) = 1.0$ bit

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Solution: Take the **expected** (average) information!

Entropy: Expected Information

Definition: Entropy Formula

$$H(X) = \mathbb{E}[I(X)] = -\sum_i p(x_i) \log_2 p(x_i)$$

Entropy $=$ Expected amount of information per observation

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Seattle weather calculation:

$$\begin{align} H &= -p(\text{rain})\log_2 p(\text{rain}) - p(\text{cloudy})\log_2 p(\text{cloudy}) \tag{1}\\ &\quad - p(\text{sunny})\log_2 p(\text{sunny}) - p(\text{snow})\log_2 p(\text{snow}) \tag{2}\\ &= -0.5\log_2(0.5) - 0.3\log_2(0.3) - 0.15\log_2(0.15) - 0.05\log_2(0.05) \tag{3}\\ &= 0.5(1.0) + 0.3(1.74) + 0.15(2.74) + 0.05(4.32) \tag{4}\\ &= 0.5 + 0.52 + 0.41 + 0.22 = \mathbf{1.65} \text{ bits} \tag{5} \end{align}$$

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Key insight: Entropy ranges from 0 (certain) to $\log_2(n)$ (uniform over n outcomes)

Entropy in Decision Trees: The Connection

Why do we care about entropy in ML?

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Example: Decision Tree Goal

We want to split data into **pure** subsets where we can make confident predictions.

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This is exactly what **Information Gain** measures.

Entropy

Statistical measure to characterize the (im)purity of examples

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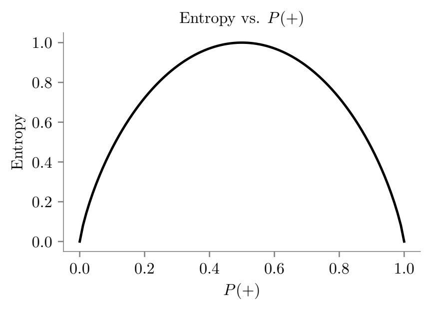
$H(X) = -\sum_{i=1}^{k} p(x_i) \log_2 p(x_i)$

Notebook: entropy.html



Towards biggest estimated performance gain

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Day	Outlook	Temp	Humidity	Windy	Play
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D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
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- Can we use Outlook as the root node?
- When Outlook is overcast, we always Play and thus no "disagreement"

Information Gain

Reduction in entropy by partitioning examples (S) on attribute A

$$\text{Gain}(S, A) \equiv \text{Entropy}(S) - \sum_{v \in \text{Values}(A)} \frac{|S_v|}{|S|} \text{Entropy}(S_v)$$

Pop Quiz #1

Quick Question!

What does entropy measure in the context of decision trees?

A) The depth of the tree

Pop Quiz #2

Quick Question!

What does entropy measure in the context of decision trees?

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B) The impurity or "disagreement" in a set of examples

Pop Quiz #3

Quick Question!

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C) The number of features in the dataset

Pop Quiz #4

Quick Question!

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D) The accuracy of the tree

Pop Quiz #5

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Pop Quiz #6

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A) The depth of the tree
B) The impurity or "disagreement" in a set of examples
C) The number of features in the dataset
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Answer: B) The impurity or "disagreement" in a set of examples - Higher entropy means more mixed classes, lower entropy means more pure subsets.

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    - For each value (v) of A

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    - Examples_v: subset of examples that $A = v$

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    - Examples_v: subset of examples that A = v
    - If Examples_v is empty: add leaf with label = most common value of Target Attribute

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  - A $\leftarrow$ attribute from Attributes which best classifies Examples
  - Root $\leftarrow$ A
  - For each value (v) of A
    - Add new tree branch : A = v
    - Examples_v: subset of examples that A = v
    - If Examples_v is empty: add leaf with label = most common value of Target Attribute
    - Else: ID3 (Examples_v, Target attribute, Attributes - A)

Learnt Decision Tree

$\boxed{\text{Root Node (empty)}}$

Training Data

Day	Outlook	Temp	Humidity	Windy	Play
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

Entropy calculated

We have 14 examples in S: 5 No, 9 Yes

$$
\begin{aligned}
\text{Entropy}(S) &= -p_{\text{No}} \log_2 p_{\text{No}} - p_{\text{Yes}} \log_2 p_{\text{Yes}} \\
&= -\frac{5}{14} \log_2 \left(\frac{5}{14}\right) - \frac{9}{14} \log_2 \left(\frac{9}{14}\right) = 0.940
\end{aligned}
$$

Information Gain for Outlook

Outlook	**Play**
Sunny	No
Sunny	No
Overcast	Yes
Rain	Yes
Rain	Yes
Rain	No
Overcast	Yes
Sunny	No
Sunny	Yes
Rain	Yes
Sunny	Yes
Overcast	Yes
Overcast	Yes
Rain	No

Information Gain for Outlook

Information Gain for Outlook

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes

We have 2 Yes, 3 No Entropy $= -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$

Information Gain for Outlook

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes

We have 2 Yes, 3 No Entropy $= -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$

Information Gain for Outlook

Outlook	**Play**
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes

We have 2 Yes, 3 No Entropy $= -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$

Outlook	**Play**
Overcast	Yes
Overcast	Yes
Overcast	Yes
Overcast	Yes

We have 4 Yes, 0 No Entropy $= 0$ (pure subset)

Information Gain for Outlook

Outlook	**Play**
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes

We have 2 Yes, 3 No Entropy $= -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$

Outlook	**Play**
Overcast	Yes
Overcast	Yes
Overcast	Yes
Overcast	Yes

We have 4 Yes, 0 No Entropy $= 0$ (pure subset)

Information Gain for Outlook

Outlook	Play
Sunny	No
Sunny	No
Sunny	No
Sunny	Yes
Sunny	Yes

We have 2 Yes, 3 No Entropy $= -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$

Outlook	Play
Overcast	Yes
Overcast	Yes
Overcast	Yes
Overcast	Yes

We have 4 Yes, 0 No Entropy $= 0$ (pure subset)

Outlook	Play
Rain	Yes
Rain	Yes
Rain	No
Rain	Yes
Rain	No

We have 3 Yes, 2 No Entropy $= -\frac{3}{5}\log_2\left(\frac{3}{5}\right) - \frac{2}{5}\log_2\left(\frac{2}{5}\right) = 0.971$

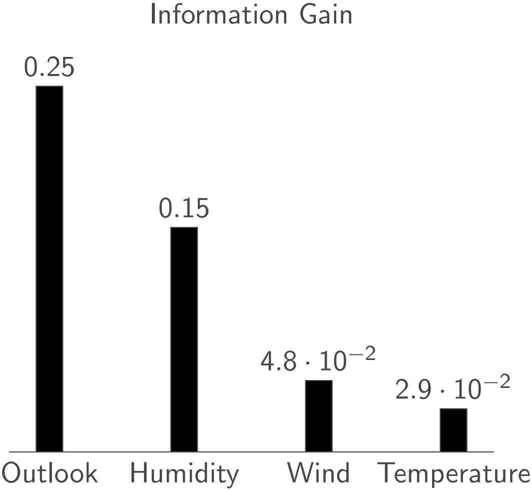
Information Gain

$$\text{Gain}(S, \text{Outlook}) = \text{Entropy}(S) - \sum_{v \in \{\text{Rain, Sunny, Overcast}\}} \frac{|S_v|}{|S|} \text{Entropy}(S_v)$$

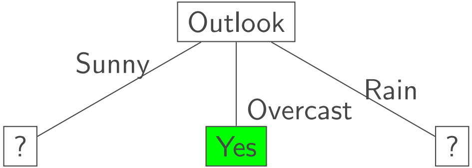
$$\text{Gain}(S, \text{Outlook}) = \text{Entropy}(S) - \frac{5}{14}\,\text{Entropy}(S_{\text{Sunny}}) - \frac{4}{14}\,\text{Entropy}(S_{\text{Overc}}$$

$$= 0.940 - \frac{5}{14} \times 0.971 - \frac{4}{14} \times 0 - \frac{5}{14} \times 0.971 = 0.940 - 0.347 - 0 - 0.347 = 0.2$$

Information Gain



Learnt Decision Tree



Calling ID3 on Outlook=Sunny

Day	**Temp**	**Humidity**	**Windy**	**Play**
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

Calling ID3 on Outlook=Sunny

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

- Gain($S_{\text{Outlook=Sunny}}$, Temp) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(0 Yes, 2 No) -(2/5)*Entropy(1 Yes, 1 No) - (1/5)*Entropy(1 Yes, 0 No)

Calling ID3 on Outlook=Sunny

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

- Gain($S_{\text{Outlook=Sunny}}$, Temp) $=$ Entropy(2 Yes, 3 No) - (2/5)*Entropy(0 Yes, 2 No) -(2/5)*Entropy(1 Yes, 1 No) - (1/5)*Entropy(1 Yes, 0 No)

Calling ID3 on Outlook=Sunny

Day	**Temp**	**Humidity**	**Windy**	**Play**
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

- Gain($S_{\text{Outlook=Sunny}}$, Temp) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(0 Yes, 2 No) -(2/5)*Entropy(1 Yes, 1 No) - (1/5)*Entropy(1 Yes, 0 No)
- Gain($S_{\text{Outlook=Sunny}}$, Humidity) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(2 Yes, 0 No) -(3/5)*Entropy(0 Yes, 3 No) $\Longrightarrow$ **maximum possible for the set**

Calling ID3 on Outlook=Sunny

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

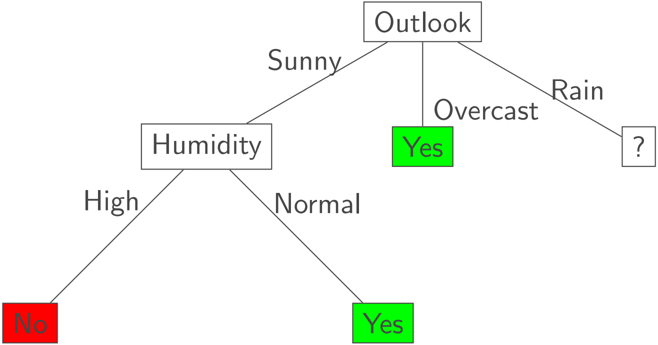
- Gain($S_{\text{Outlook=Sunny}}$, Temp) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(0 Yes, 2 No) -(2/5)*Entropy(1 Yes, 1 No) - (1/5)*Entropy(1 Yes, 0 No)
- Gain($S_{\text{Outlook=Sunny}}$, Humidity) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(2 Yes, 0 No) -(3/5)*Entropy(0 Yes, 3 No) $\implies$ **maximum possible for the set**

Calling ID3 on Outlook=Sunny

Day	Temp	Humidity	Windy	Play
D1	Hot	High	Weak	No
D2	Hot	High	Strong	No
D8	Mild	High	Weak	No
D9	Cool	Normal	Weak	Yes
D11	Mild	Normal	Strong	Yes

- Gain($S_{\text{Outlook=Sunny}}$, Temp) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(0 Yes, 2 No) -(2/5)*Entropy(1 Yes, 1 No) - (1/5)*Entropy(1 Yes, 0 No)
- Gain($S_{\text{Outlook=Sunny}}$, Humidity) = Entropy(2 Yes, 3 No) - (2/5)*Entropy(2 Yes, 0 No) -(3/5)*Entropy(0 Yes, 3 No) $\implies$ **maximum possible for the set**
- Gain($S_{\text{Outlook=Sunny}}$, Windy) = Entropy(2 Yes, 3 No) - (3/5)*Entropy(1 Yes, 2 No) -(2/5)*Entropy(1 Yes, 1 No)

Learnt Decision Tree

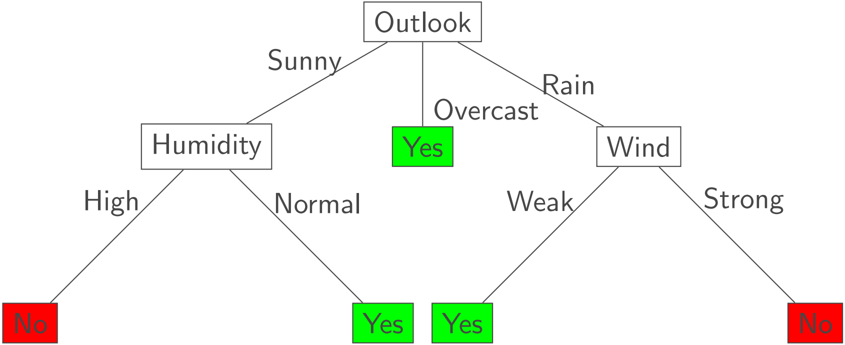


Calling ID3 on (Outlook=Rain)

Day	Temp	Humidity	Windy	Play
D4	Mild	High	Weak	Yes
D5	Cool	Normal	Weak	Yes
D6	Cool	Normal	Strong	No
D10	Mild	Normal	Weak	Yes
D14	Mild	High	Strong	No

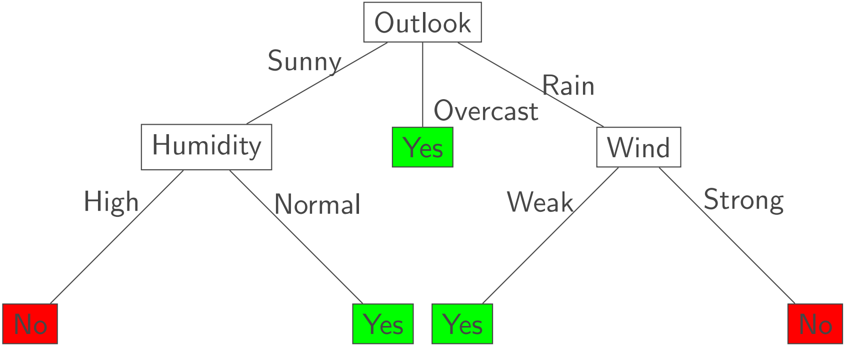
- The attribute Windy gives the highest information gain

Learnt Decision Tree



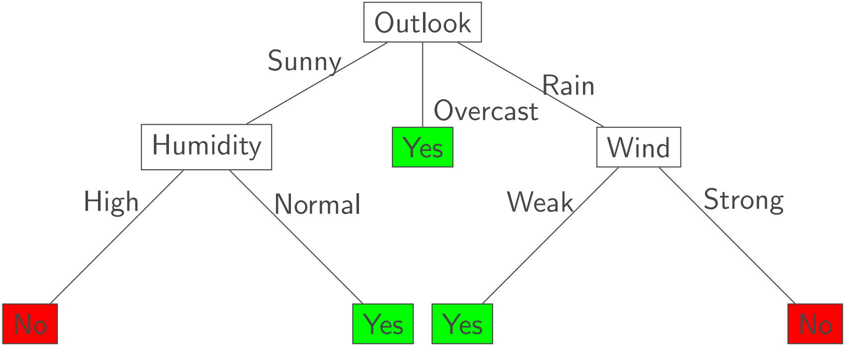
Prediction for Decision Tree

Just walk down the tree!



Prediction for Decision Tree

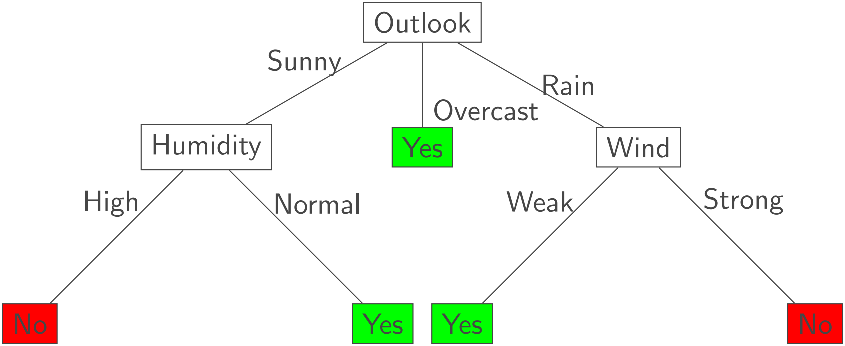
Just walk down the tree!



Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

Prediction for Decision Tree

Just walk down the tree!



Prediction for <High Humidity, Strong Wind, Sunny Outlook, Hot Temp> is ?

No

Limiting Tree Depth

Definition: Depth-Limited Trees

When depth limit is reached, assign the **most common class** in that path as the leaf node prediction.

Limiting Tree Depth

Definition: Depth-Limited Trees

When depth limit is reached, assign the **most common class** in that path as the leaf node prediction.

- **Depth-0 tree** (no decisions):

Limiting Tree Depth

Definition: Depth-Limited Trees

When depth limit is reached, assign the **most common class** in that path as the leaf node prediction.

- **Depth-0 tree** (no decisions):
  - Always predict the most common class

Limiting Tree Depth

Definition: Depth-Limited Trees

When depth limit is reached, assign the **most common class** in that path as the leaf node prediction.

- **Depth-0 tree** (no decisions):
  - Always predict the most common class
  - For our dataset: Always predict **Yes**

Limiting Tree Depth

Definition: Depth-Limited Trees

When depth limit is reached, assign the **most common class** in that path as the leaf node prediction.

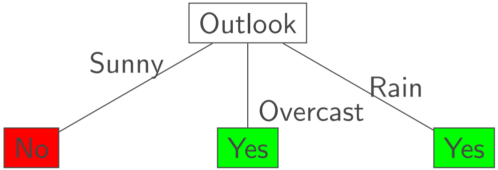
- **Depth-0 tree** (no decisions):
  - Always predict the most common class
  - For our dataset: Always predict **Yes**

Limiting Tree Depth

Definition: Depth-Limited Trees

When depth limit is reached, assign the **most common class** in that path as the leaf node prediction.

- **Depth-0 tree** (no decisions):
  - Always predict the most common class
  - For our dataset: Always predict **Yes**
- **Depth-1 tree** (single decision):



Pop Quiz #7

Quick Question!

In the tennis dataset, why did "Outlook" have the highest information gain?

A) It was the first feature in the dataset

Pop Quiz #8

Quick Question!

In the tennis dataset, why did "Outlook" have the highest information gain?

A) It was the first feature in the dataset

B) When Outlook=Overcast, all examples have Play=Yes (pure subset)

Pop Quiz #9

Quick Question!

In the tennis dataset, why did "Outlook" have the highest information gain?

A) It was the first feature in the dataset

B) When Outlook=Overcast, all examples have Play=Yes (pure subset)

C) It has the most possible values

Pop Quiz #10

Quick Question!

In the tennis dataset, why did "Outlook" have the highest information gain?

A) It was the first feature in the dataset

B) When Outlook=Overcast, all examples have Play=Yes (pure subset)

C) It has the most possible values

D) It was chosen randomly

Pop Quiz #11

Quick Question!

In the tennis dataset, why did "Outlook" have the highest information gain?

A) It was the first feature in the dataset

B) When Outlook=Overcast, all examples have Play=Yes (pure subset)

C) It has the most possible values

D) It was chosen randomly

Pop Quiz #12

Quick Question!

In the tennis dataset, why did "Outlook" have the highest information gain?

A) It was the first feature in the dataset
B) When Outlook=Overcast, all examples have Play=Yes (pure subset)
C) It has the most possible values
D) It was chosen randomly

Answer: B) When Outlook=Overcast, all examples have Play=Yes - This creates a pure subset with entropy=0, maximizing information gain.

Modified Dataset

Day	Outlook	Temp	Humidity	Wind	Minutes Played
D1	Sunny	Hot	High	Weak	20
D2	Sunny	Hot	High	Strong	24
D3	Overcast	Hot	High	Weak	40
D4	Rain	Mild	High	Weak	50
D5	Rain	Cool	Normal	Weak	60
D6	Rain	Cool	Normal	Strong	10
D7	Overcast	Cool	Normal	Strong	4
D8	Sunny	Mild	High	Weak	10
D9	Sunny	Cool	Normal	Weak	60
D10	Rain	Mild	Normal	Weak	40
D11	Sunny	Mild	High	Strong	45
D12	Overcast	Mild	High	Strong	40
D13	Overcast	Hot	Normal	Weak	35
D14	Rain	Mild	High	Strong	20

Measure of Impurity for Regression?

Measure of Impurity for Regression?

Measure of Impurity for Regression?

- Any guesses?

Measure of Impurity for Regression?

- Any guesses?

Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error

Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error

Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error
- $\text{MSE}(S) = 311.34$

Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error
- $\text{MSE}(S) = 311.34$

Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error
- $\mathrm{MSE}(S) = 311.34$
- What about splitting criterion for regression?

Measure of Impurity for Regression?

- Any guesses?
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- $\text{MSE}(S) = 311.34$
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Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error
- $\text{MSE}(S) = 311.34$
- What about splitting criterion for regression?
- **MSE Reduction** (not Information Gain!)

Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error
- $\text{MSE}(S) = 311.34$
- What about splitting criterion for regression?
- **MSE Reduction** (not Information Gain!)

Measure of Impurity for Regression?

- Any guesses?
- Mean Squared Error
- $\text{MSE}(S) = 311.34$
- What about splitting criterion for regression?
- **MSE Reduction** (not Information Gain!)
- $\text{MSE Reduction} = \text{MSE}(S) - \sum_v \frac{|S_v|}{|S|} \text{MSE}(S_v)$

Gain by splitting on Wind

Gain by splitting on Wind

Wind	**Minutes Played**
Weak	20
Strong	24
Weak	40
Weak	50
Weak	60
Strong	10
Strong	4
Weak	10
Weak	60
Weak	40
Strong	45
Strong	40
Weak	35
Strong	20

MSE(S)=311.34

Gain by splitting on Wind

Wind	Minutes Played
Weak	20
Strong	24
Weak	40
Weak	50
Weak	60
Strong	10
Strong	4
Weak	10
Weak	60
Weak	40
Strong	45
Strong	40
Weak	35
Strong	20

MSE(S)=311.34

Wind	Minutes Played
Weak	20
Weak	40
Weak	50
Weak	60
Weak	10
Weak	60
Weak	40
Weak	35

$\mathrm{MSE}(S_{\mathrm{Wind=Weak}}) = 277$, Weight $= \frac{8}{14}$

Wind	Minutes Played
Strong	24
Strong	10
Strong	4
Strong	45
Strong	40
Strong	20

$\mathrm{MSE}(S_{\mathrm{Wind=Strong}}) = 218$, Weight $= \frac{6}{14}$

MSE Reduction Calculation

Correct calculation for Wind split:

$$\text{MSE Reduction} = \text{MSE}(S) - \text{Weighted Average MSE}$$

$$= 311.34 - \left[\frac{8}{14} \times 277 + \frac{6}{14} \times 218\right] = 311.34 - [158.857 + 93.429] = 311.$$

Key insight: MSE Reduction > 0 means the split improves our model!

For regression: Use MSE Reduction, NOT Information Gain!

Pop Quiz #13

Quick Question!

For regression trees, what criterion do we use instead of Information Gain?

A) Information Gain

Pop Quiz #14

Quick Question!

For regression trees, what criterion do we use instead of Information Gain?

A) Information Gain

B) Gini Impurity

Pop Quiz #15

Quick Question!

For regression trees, what criterion do we use instead of Information Gain?

A) Information Gain
B) Gini Impurity
C) Mean Squared Error (MSE) Reduction

Pop Quiz #16

Quick Question!

For regression trees, what criterion do we use instead of Information Gain?

A) Information Gain
B) Gini Impurity
C) Mean Squared Error (MSE) Reduction
D) Accuracy

Pop Quiz #17

Quick Question!

For regression trees, what criterion do we use instead of Information Gain?

A) Information Gain
B) Gini Impurity
C) Mean Squared Error (MSE) Reduction
D) Accuracy

Pop Quiz #18

Quick Question!

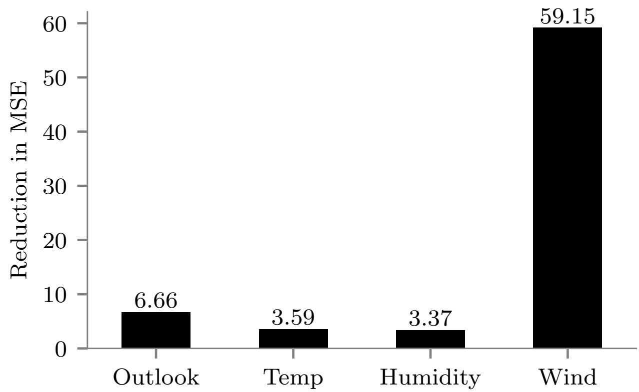
For regression trees, what criterion do we use instead of Information Gain?

A) Information Gain
B) Gini Impurity
C) Mean Squared Error (MSE) Reduction
D) Accuracy

Answer: C) Mean Squared Error (MSE) Reduction - For regression, we minimize MSE instead of maximizing information gain.

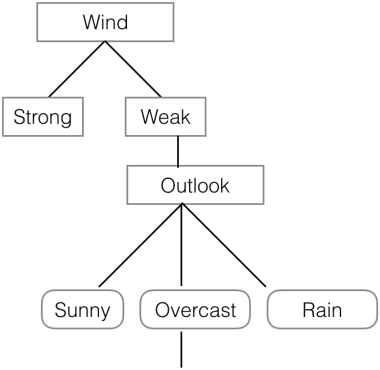
MSE Reduction for Regression Trees

Notebook: decision-tree-real-output.html



Learnt Tree

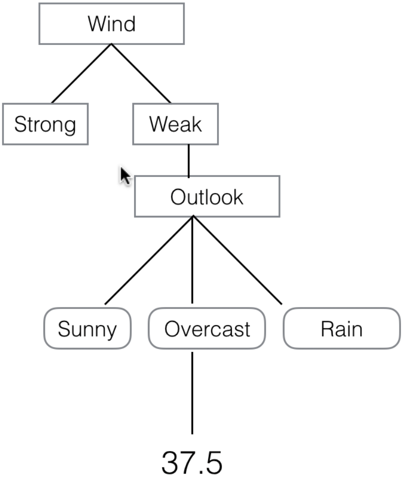
Assume a tree like this is learnt ...



	Day	Outlook	Temp	Humidity	Wind	Minutes Played
2	D3	Overcast	Hot	High	Weak	40
12	D13	Overcast	Hot	Normal	Weak	35

Learnt Tree

Method 1
Mins Played=(40+35)/2



Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66, 76, 85

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66, 76, 85
- Calculate the weighted impurity for each split

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- How do you find splits?
- Sort by attribute
- Find potential split points (midpoints).
- For the above example, we have 5 potential splits: 44, 54, 66, 76, 85
- Calculate the weighted impurity for each split
- Choose the split with the lowest impurity

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 44

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 44
- LHS has 1 No and 0 Yes; RHS has 3 Yes and 2 No

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 44
- LHS has 1 No and 0 Yes; RHS has 3 Yes and 2 No
- Entropy for LHS $= 0$, Entropy for RHS $= 0.971$

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 44
- LHS has 1 No and 0 Yes; RHS has 3 Yes and 2 No
- Entropy for LHS $= 0$, Entropy for RHS $= 0.971$
- Weighted Entropy $= 0.971*5/6 = 0.808$

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 54

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 54
- LHS has 2 No and 0 Yes; RHS has 3 Yes and 1 No

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 54
- LHS has 2 No and 0 Yes; RHS has 3 Yes and 1 No
- Entropy for LHS $= 0$, Entropy for RHS $= 0.811$

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 54
- LHS has 2 No and 0 Yes; RHS has 3 Yes and 1 No
- Entropy for LHS = 0, Entropy for RHS = 0.811
- Weighted Entropy = 0.811*4/6 = 0.541

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 66

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 66
- LHS has 2 No and 1 Yes; RHS has 2 Yes and 1 No

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 66
- LHS has 2 No and 1 Yes; RHS has 2 Yes and 1 No
- Entropy for LHS = 0.918, Entropy for RHS = 0.918

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 66
- LHS has 2 No and 1 Yes; RHS has 2 Yes and 1 No
- Entropy for LHS $= 0.918$, Entropy for RHS $= 0.918$
- Weighted Entropy $= 0.918*3/6 + 0.918*3/6 = 0.918$

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 76

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 76
- LHS has 2 No and 2 Yes; RHS has 1 Yes and 1 No

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 76
- LHS has 2 No and 2 Yes; RHS has 1 Yes and 1 No
- Entropy for LHS $= 1$, Entropy for RHS $= 1$

Finding splits

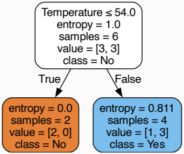
Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

- Consider split at 76
- LHS has 2 No and 2 Yes; RHS has 1 Yes and 1 No
- Entropy for LHS $= 1$, Entropy for RHS $= 1$
- Weighted Entropy $= 1*4/6 + 1*2/6 = 1$

Finding splits

Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

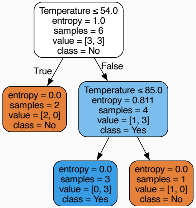
Notebook: decision-tree-real-input-discrete-output.html



Finding splits

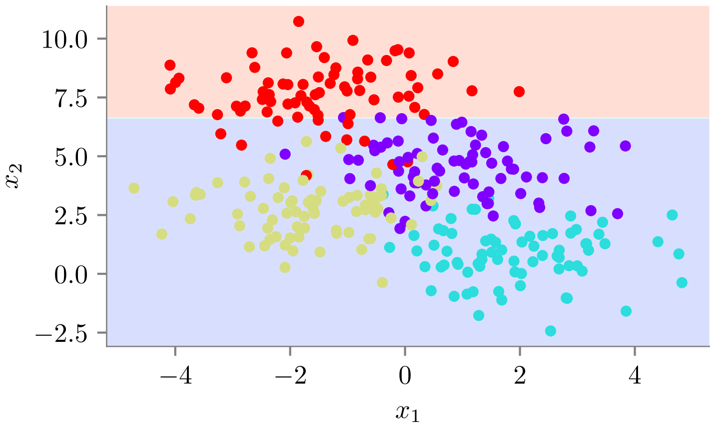
Day	Temperature	PlayTennis
D1	40	No
D2	48	No
D3	60	Yes
D4	72	Yes
D5	80	Yes
D6	90	No

Notebook: decision-tree-real-input-discrete-output.html



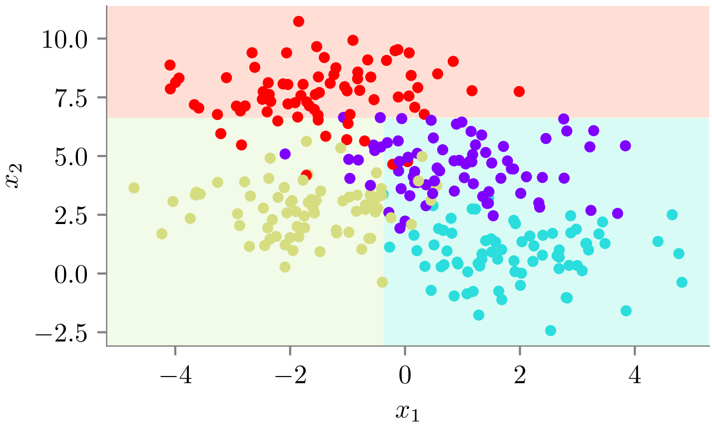
Example (DT of depth 1)

Notebook: decision-tree-real-input-discrete-output.html



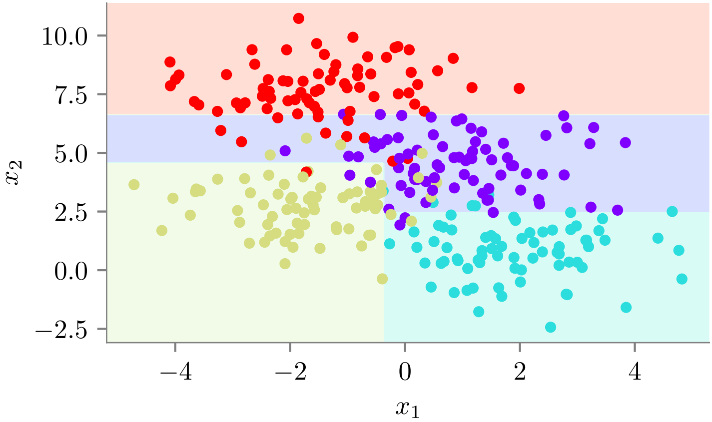
Example (DT of depth 2)

Notebook: decision-tree-real-input-discrete-output.html



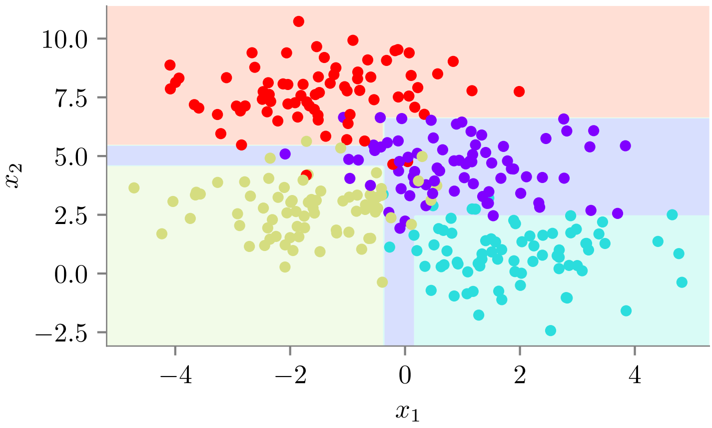
Example (DT of depth 3)

Notebook: decision-tree-real-input-discrete-output.html



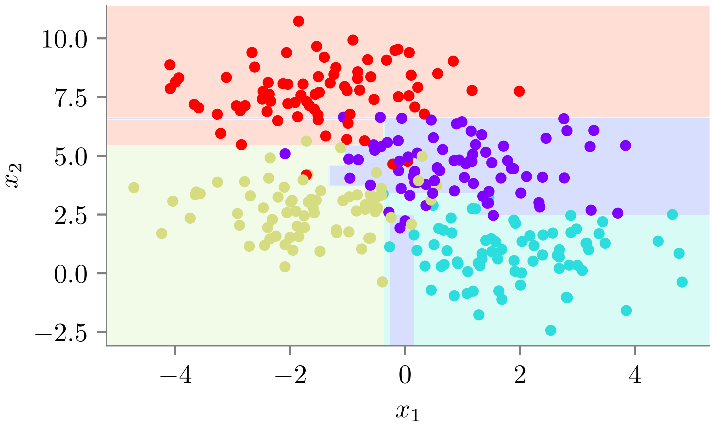
Example (DT of depth 4)

Notebook: decision-tree-real-input-discrete-output.html



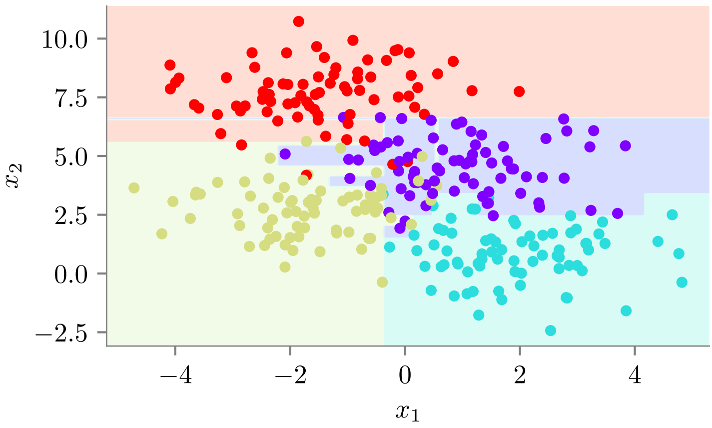
Example (DT of depth 5)

Notebook: decision-tree-real-input-discrete-output.html



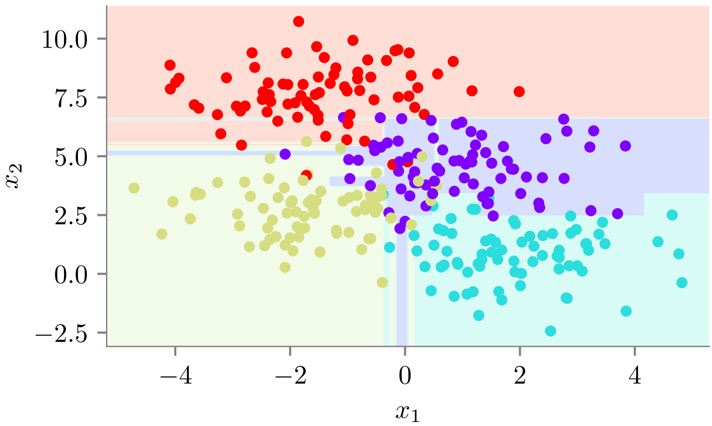
Example (DT of depth 6)

Notebook: decision-tree-real-input-discrete-output.html



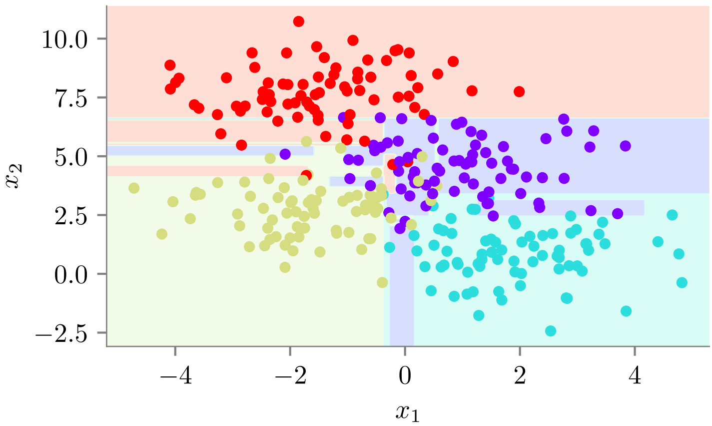
Example (DT of depth 7)

Notebook: decision-tree-real-input-discrete-output.html



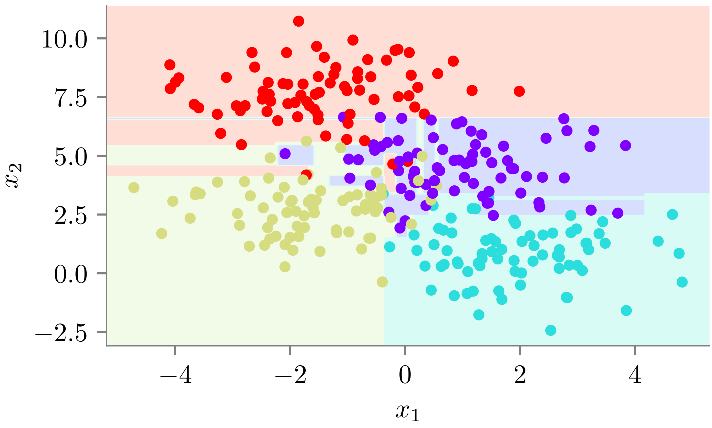
Example (DT of depth 8)

Notebook: decision-tree-real-input-discrete-output.html



Example (DT of depth 9)

Notebook: decision-tree-real-input-discrete-output.html



Pop Quiz #19

Quick Question!

When finding splits for continuous features, how do we determine candidate split points?

A) Use all feature values as split points

Pop Quiz #20

Quick Question!

When finding splits for continuous features, how do we determine candidate split points?

A) Use all feature values as split points

B) Use midpoints between consecutive sorted feature values

Pop Quiz #21

Quick Question!

When finding splits for continuous features, how do we determine candidate split points?

A) Use all feature values as split points

B) Use midpoints between consecutive sorted feature values

C) Use random values within the feature range

Pop Quiz #22

Quick Question!

When finding splits for continuous features, how do we determine candidate split points?

A) Use all feature values as split points
B) Use midpoints between consecutive sorted feature values
C) Use random values within the feature range
D) Use only the minimum and maximum values

Pop Quiz #23

Quick Question!

When finding splits for continuous features, how do we determine candidate split points?

A) Use all feature values as split points
B) Use midpoints between consecutive sorted feature values
C) Use random values within the feature range
D) Use only the minimum and maximum values

Pop Quiz #24

Quick Question!

When finding splits for continuous features, how do we determine candidate split points?

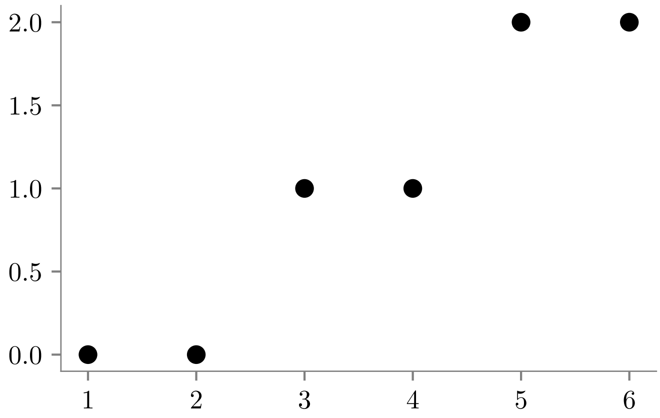
A) Use all feature values as split points
B) Use midpoints between consecutive sorted feature values
C) Use random values within the feature range
D) Use only the minimum and maximum values

Answer: B) Use midpoints between consecutive sorted feature values - This ensures we test all meaningful boundaries between different class regions.

Example 1

Let us consider the dataset given below

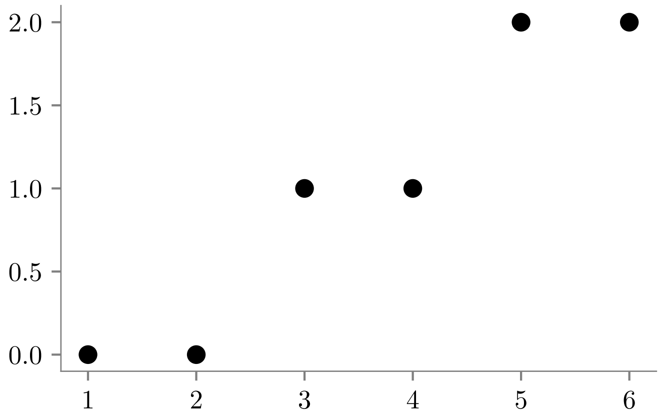
Notebook: decision-tree-real-input-real-output.html



Example 1

What would be the prediction for decision tree with depth 0?

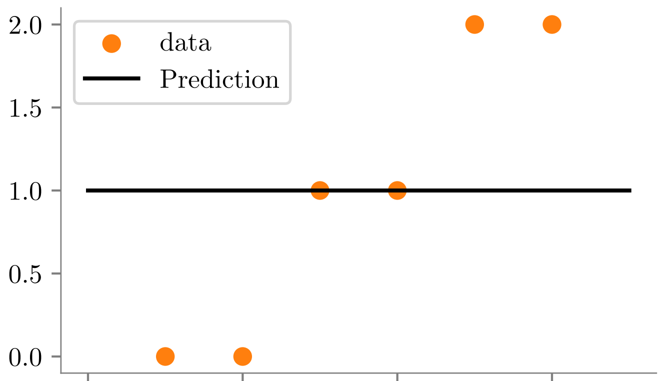
Notebook: decision-tree-real-input-real-output.html



Example 1

Prediction for decision tree with depth 0.
Horizontal dashed line shows the predicted Y value. It is the average of Y values of all datapoints.

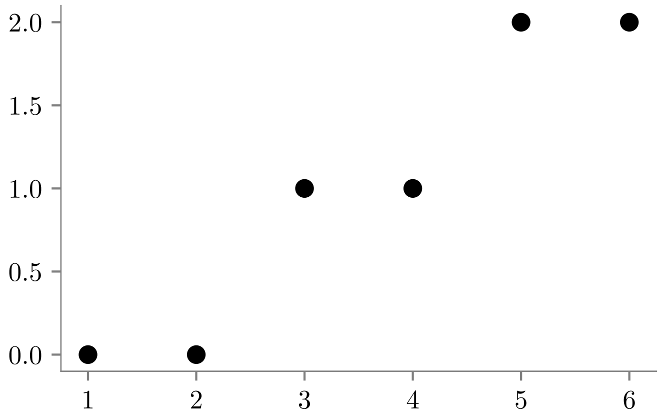
Notebook: decision-tree-real-input-real-output.html



Example 1

What would be the decision tree with depth 1?

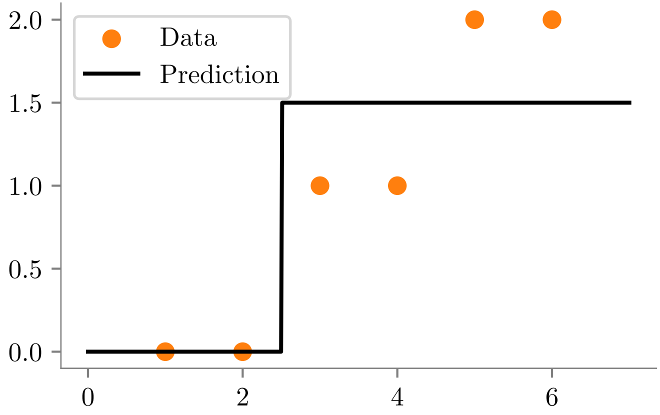
Notebook: decision-tree-real-input-real-output.html



Example 1

Decision tree with depth 1

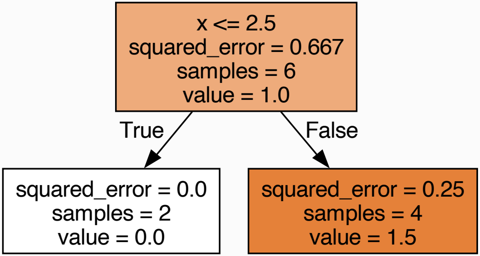
Notebook: decision-tree-real-input-real-output.html



Example 1

The Decision Boundary

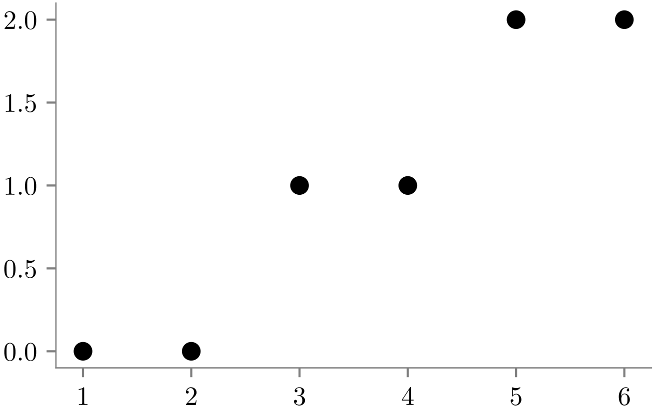
Notebook: decision-tree-real-input-real-output.html



Example 1

What would be the decision tree with depth 2 ?

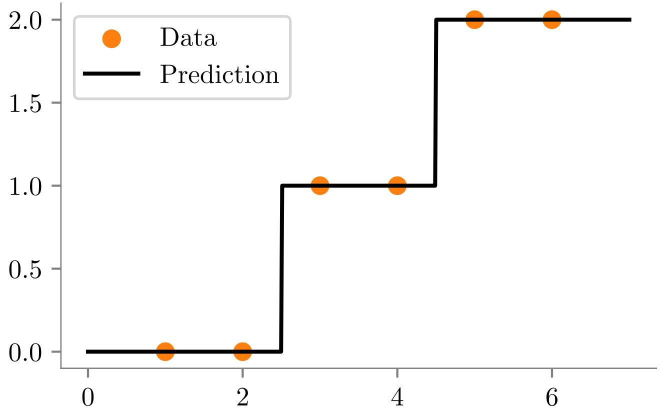
Notebook: decision-tree-real-input-real-output.html



Example 1

Decision tree with depth 2

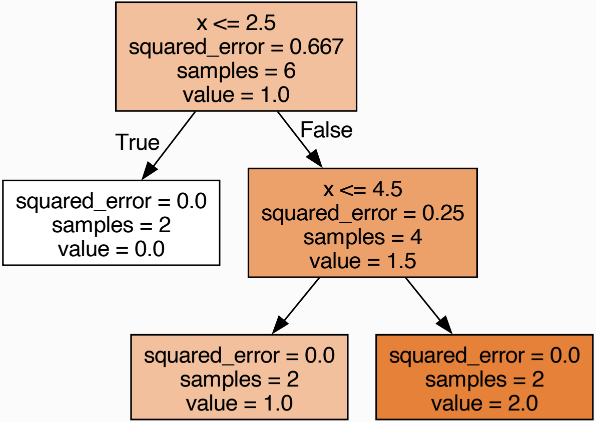
Notebook: decision-tree-real-input-real-output.html



Example 1

The Decision Boundary

Notebook: decision-tree-real-input-real-output.html



Objective Function for Regression Trees

Feature is denoted by X and target by Y.
Let the split be at $X = s$.
Define regions: $R_1 = \{x : x \leq s\}$ and $R_2 = \{x : x > s\}$.

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For each region, compute the mean prediction:
$c_1 = \frac{1}{|R_1|} \sum_{x_i \in R_1} y_i$
$c_2 = \frac{1}{|R_2|} \sum_{x_i \in R_2} y_i$

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The loss function is:

$$\text{Loss}(s) = \sum_{x_i \in R_1} (y_i - c_1)^2 + \sum_{x_i \in R_2} (y_i - c_2)^2$$

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Our objective is to find the optimal split:

Algorithm: Finding the Optimal Split

1. Sort all data points (x_i, y_i) in increasing order of x_i.

Algorithm: Finding the Optimal Split

1. Sort all data points (x_i, y_i) in increasing order of x_i.
2. Evaluate the loss function for all candidate splits:

$$s = \tfrac{x_i + x_{i+1}}{2} \text{ for } i = 1, 2, \ldots, n-1$$

3. Select the split s^* that minimizes the loss function.

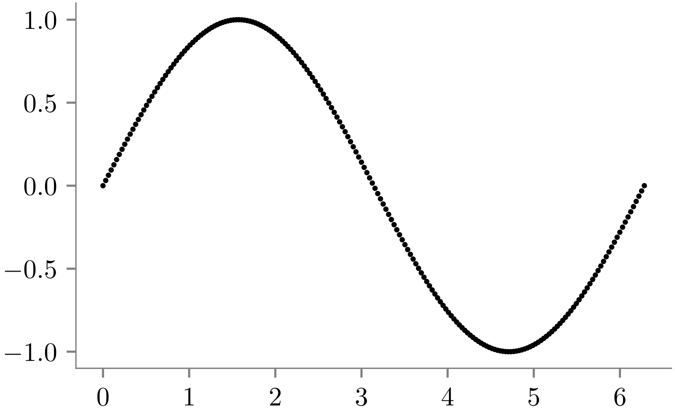
A Question!

Draw a regression tree for $Y = \sin(X)$, $0 \leq X \leq 2\pi$

A Question!

Dataset of Y = sin(X), $0 \leq X \leq 7$ with 10,000 points

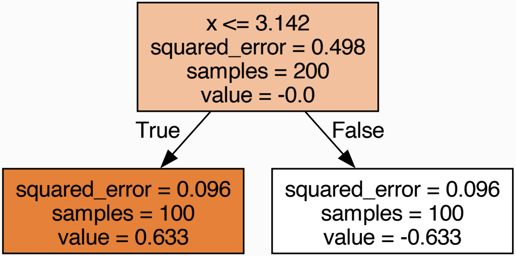
Notebook: decision-tree-real-input-real-output.html



A Question!

Regression tree of depth 1

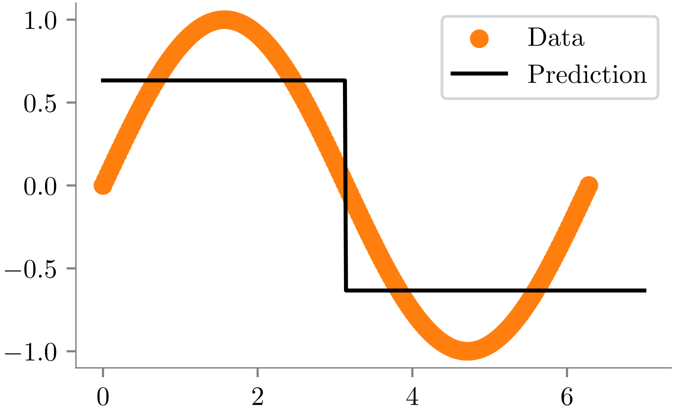
Notebook: decision-tree-real-input-real-output.html



A Question!

Decision Boundary

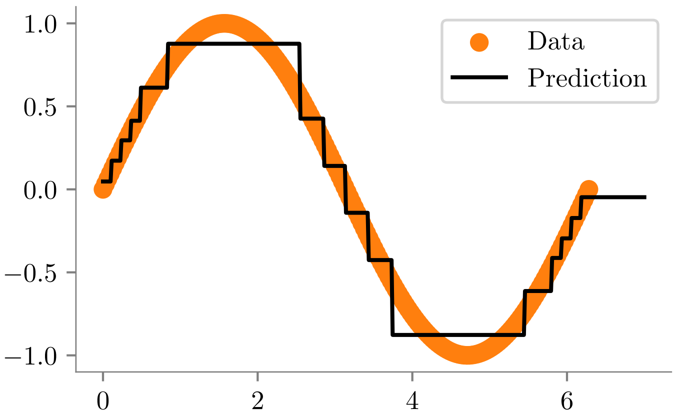
Notebook: decision-tree-real-input-real-output.html



A Question!

Regression tree with no depth limit is too big to fit in a slide.
It has of depth 4. The decision boundaries are in figure below.

Notebook: decision-tree-real-input-real-output.html



Pop Quiz #25

Quick Question!

What is the prediction function for a regression tree leaf node?

A) The median of target values in that region

Pop Quiz #26

Quick Question!

What is the prediction function for a regression tree leaf node?

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B) The mode of target values in that region

Pop Quiz #27

Quick Question!

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Pop Quiz #28

Quick Question!

What is the prediction function for a regression tree leaf node?

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B) The mode of target values in that region

C) The mean of target values in that region

D) A linear function of the features

Pop Quiz #29

Quick Question!

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A) The median of target values in that region
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C) The mean of target values in that region
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Pop Quiz #30

Quick Question!

What is the prediction function for a regression tree leaf node?

A) The median of target values in that region
B) The mode of target values in that region
C) The mean of target values in that region
D) A linear function of the features

Answer: C) The mean of target values in that region - Each leaf predicts the average target value of training samples that reach that leaf.

The Problem: Overfitting in Decision Trees

- **Unpruned trees**: Can grow very deep and complex

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- **Perfect training accuracy**: Each leaf contains single training example

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- **But**: Poor generalization to new data
- **Symptoms**:
    - High training accuracy, low test accuracy
    - Very deep trees with many leaves
    - Rules that are too specific to training data
- **Solution**: Pruning to control model complexity

Pre-pruning (Early Stopping)

Stop growing tree before it becomes too complex:

- **Maximum depth**: Limit tree depth (e.g., max_depth = 5)

Advantages: Simple, computationally efficient
Disadvantages: May stop too early, miss good splits later

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- **Minimum samples per leaf**: Ensure each leaf has $\geq$ M samples
- **Maximum features**: Consider only subset of features at each split
- **Minimum impurity decrease**: Only split if improvement ¿ threshold

Advantages: Simple, computationally efficient
Disadvantages: May stop too early, miss good splits later

Post-pruning (Tree Simplification)

Grow full tree, then remove unnecessary branches:

- **Algorithm**:

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- **Cost Complexity Pruning**: Minimize Error $+ \alpha \times$ Tree Size

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- **Cost Complexity Pruning**: Minimize Error $+ \alpha \times$ Tree Size
- **Advantages**: More thorough, can recover from early stopping mistakes
- **Disadvantages**: More computationally expensive

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

- **Cost function**: $R_\alpha(T) = R(T) + \alpha|T|$

Cost Complexity Pruning Algorithm

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- **Process**:

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  - $R(T)$: Misclassification error on validation set
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- **Process**:
  1. Start with full tree ($\alpha = 0$)
  2. Gradually increase α
  3. At each α, prune branches that increase cost

Cost Complexity Pruning Algorithm

Systematic approach to find optimal tree size:

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  - α: Complexity parameter (penalty for larger trees)
- **Process**:
  1. Start with full tree ($\alpha = 0$)
  2. Gradually increase α
  3. At each α, prune branches that increase cost
  4. Select α with best cross-validation performance

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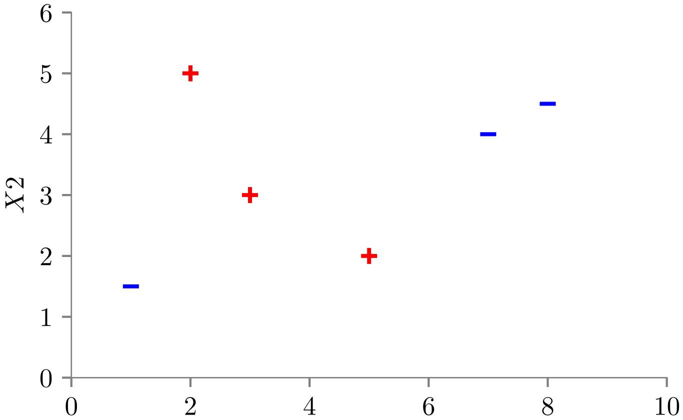

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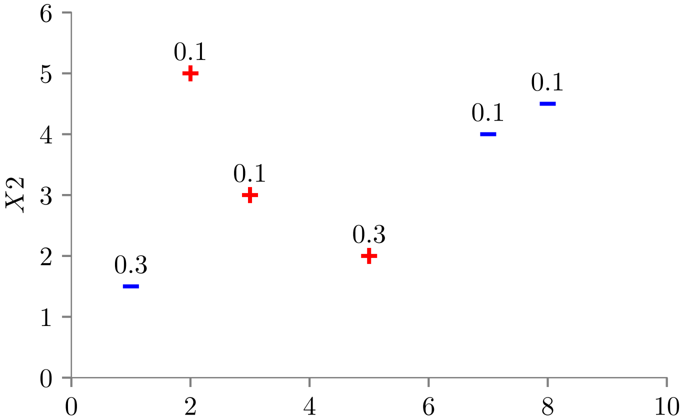
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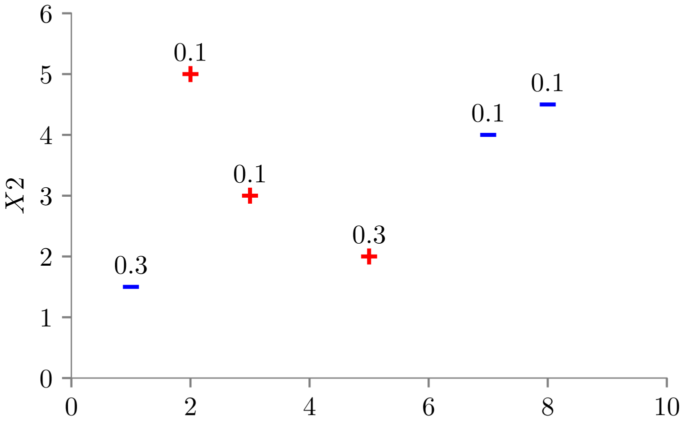
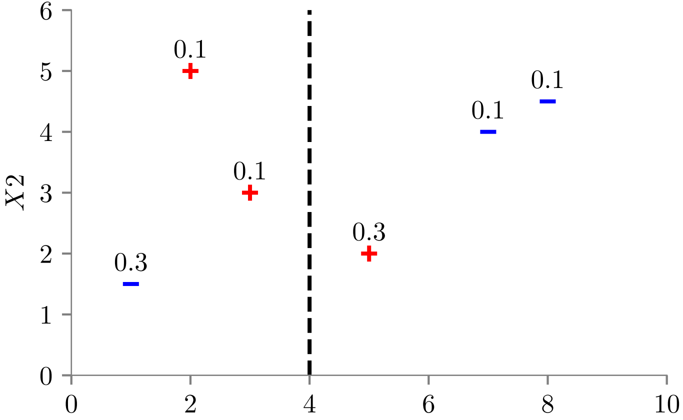
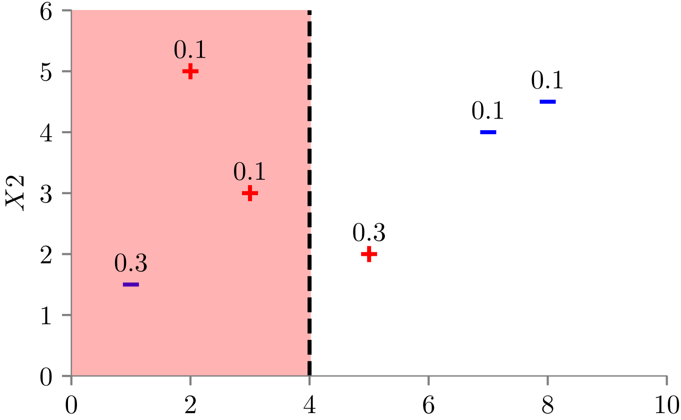


$$\text{Entropy} = -P(+)\log_2 P(+) - P(-)\log_2 P(-)$$

$$P(+) = \frac{0.1 + 0.1 + 0.3}{1} = 0.5, \quad P(-) = \frac{0.3 + 0.1 + 0.1}{1} = 0.5$$



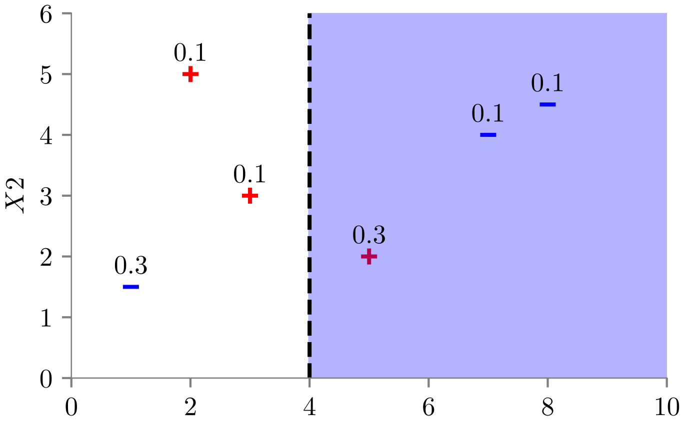
Candidate Line: $X1 = 4(X1^*)$



Entropy of $X1 \leq X1^* = E_{S(X1 < X1^*)}$

$$P(+) = \frac{0.1 + 0.1}{0.1 + 0.1 + 0.3} = \frac{2}{5}$$

$$P(-) = \frac{3}{5}$$



Entropy of $X_1 > X_1^* = E_{S(X_1 > X_1^*)}$

$$P(+) = \frac{3}{5}$$

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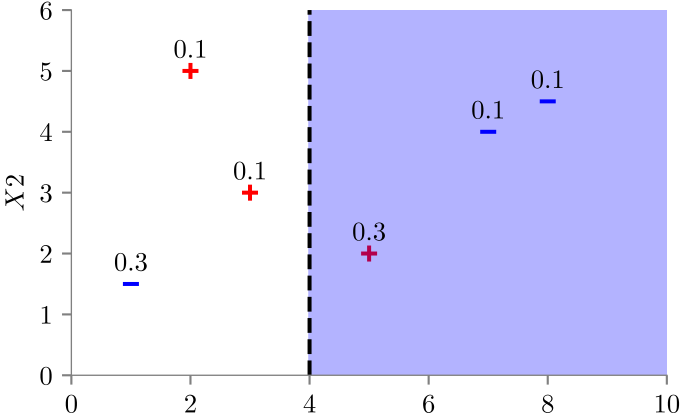

$$\mathrm{IG}(X_1 = X_1^*) = E_S - \frac{0.5}{1} \cdot E_{S(X_1 < X_1^*)} - \frac{0.5}{1} \cdot E_{S(X_1 > X_1^*)}$$